Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA

Programming Distributed Computing Platforms with COMPSs

Pol Alvarez, Javier Alvarez, Ramon Amela, Rosa M. Badia, Javier Conejero, Marc Dominguez, Jorge Ejarque, Daniele Lezzi, Francesc Lordan, Cristian Ramon-Cortes, Sergio Rodriguez

Workflows & Distributed Computing Group

29-30/01/2019

Barcelona

Outline

Day 1

- Roundtable (9:30 – 10:00): Presentation and background of participants
- Session 1 (10:00 – 10:30): Introduction to COMPSs
  - Motivation
  - Setup of tutorial environment
- Session 3 (10:30-13:00): PyCOMPSs
  - Writing Python applications
  - Coffee break (11:00 – 11:30)
  - Python Hands-on using Jupyter notebooks
- Lunch break (13:00-14:30)
- Session 4 (14:30 -15:15): How to debug COMPSs applications
- Session 5 (15:15 -16:30): Python practical session (Bring your Own Code)

- SLIDES
  - http://compss.bsc.es/releases/tutorials/tutorial-PATC_2019/

Outline

Day 2

- Session 6 (9:30-11:00): COMPSs & Java
  - Writing Java applications
  - Java Hands-on
- Coffee break (11:00 – 11:30)
- Session 7 (11:30-12:30): COMPSs Advanced Features
  - Using binaries and MPI code
  - COMPSs execution environment
  - Integration with OmpSs
- Lunch break (13:30 – 14:30)
- Session 8 (14:30-15:30): Cluster Hands-on (MareNostrum)
- Session 9 (15:30 -16:30): Practical session (Bring your Own Code)
- COMPSs Installation & Final Notes

INTRODUCTION

Motivation

- New complex architectures constantly emerging
  - With their own way of programming them
    - Fine grain: e.g. APIs to run with GPUs, NVMs (Non-Volatile Memories)
    - Coarse grain: e.g. APIs to deploy in Clouds
  - **Difficult** for programmers
    - Higher learning curve / Time To Market (TTM)
    - What about non computer scientists???
  - **Difficult** to understand what is going on during execution
    - Was it fast? Could it be even faster? Am I paying more than I should? (**Efficiency**)
  - Tune your application for each architecture (or cluster)
    - E.g. partitioning data among nodes

Motivation

- Create tools that make user's life **easier**
  - Intermediate layer: let the difficult parts to those tools
    - Act on behalf of the user
    - Distributing the work through resources
    - Dealing with architecture specifics
    - Automatically improving performance
  - Tools for visualization
    - Monitoring
    - Performance analysis

BSC vision on programming models

Applications

PM: High-level, clean, abstract interface

Power to the runtime

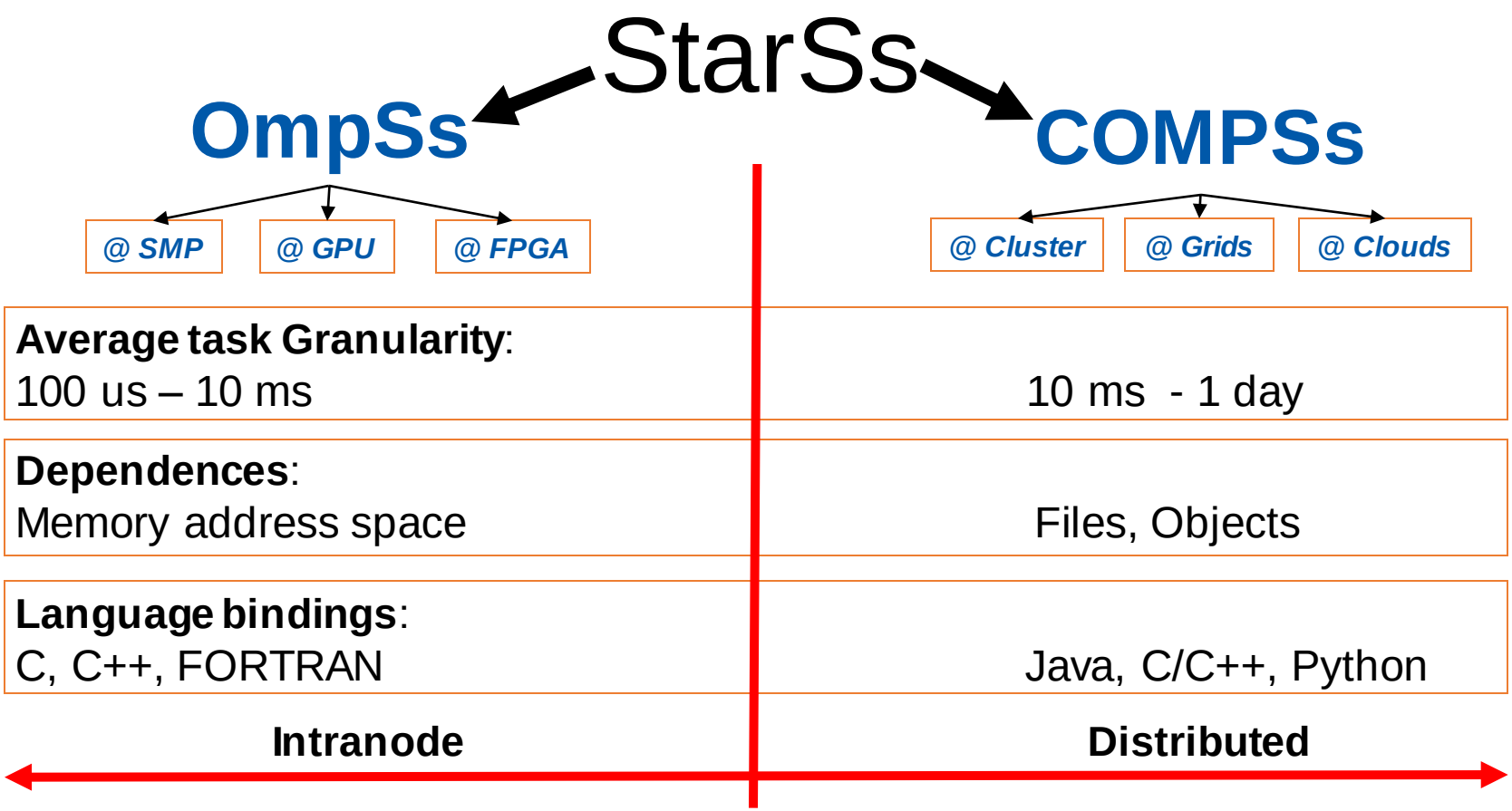
API

Program logic independent of computing platform

General purpose
Task based
Single address space

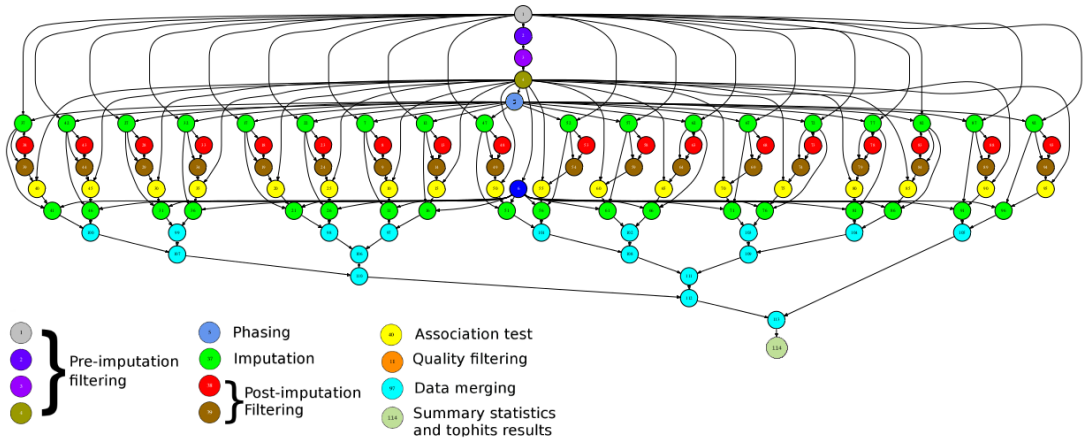
Intelligent runtime, parallelization, distribution, interoperability

BSC vision on programming models



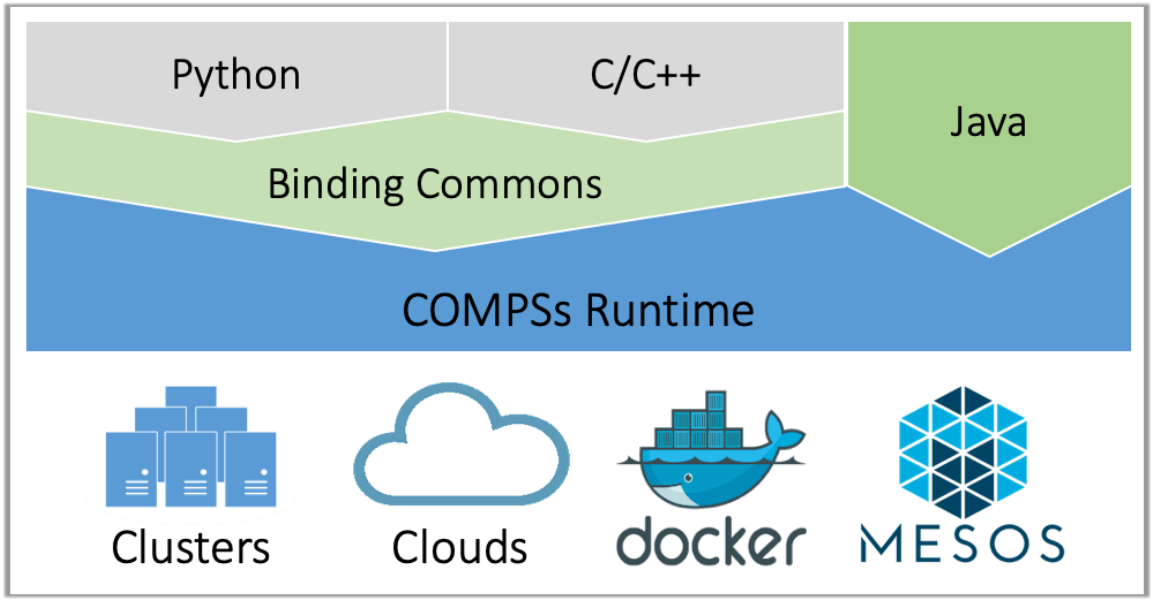
Programming with COMPSs

- Sequential programming
- General purpose programming language + annotations/hints
  - To identify tasks and directionality of data
- Task based: task is the unit of work
- Simple linear address space
- Builds a task graph at runtime that express potential concurrency
  - Implicit workflow
- Exploitation of parallelism
  - … and of distant parallelism
- Agnostic of computing platform
  - Enabled by the runtime for clusters, clouds and grids

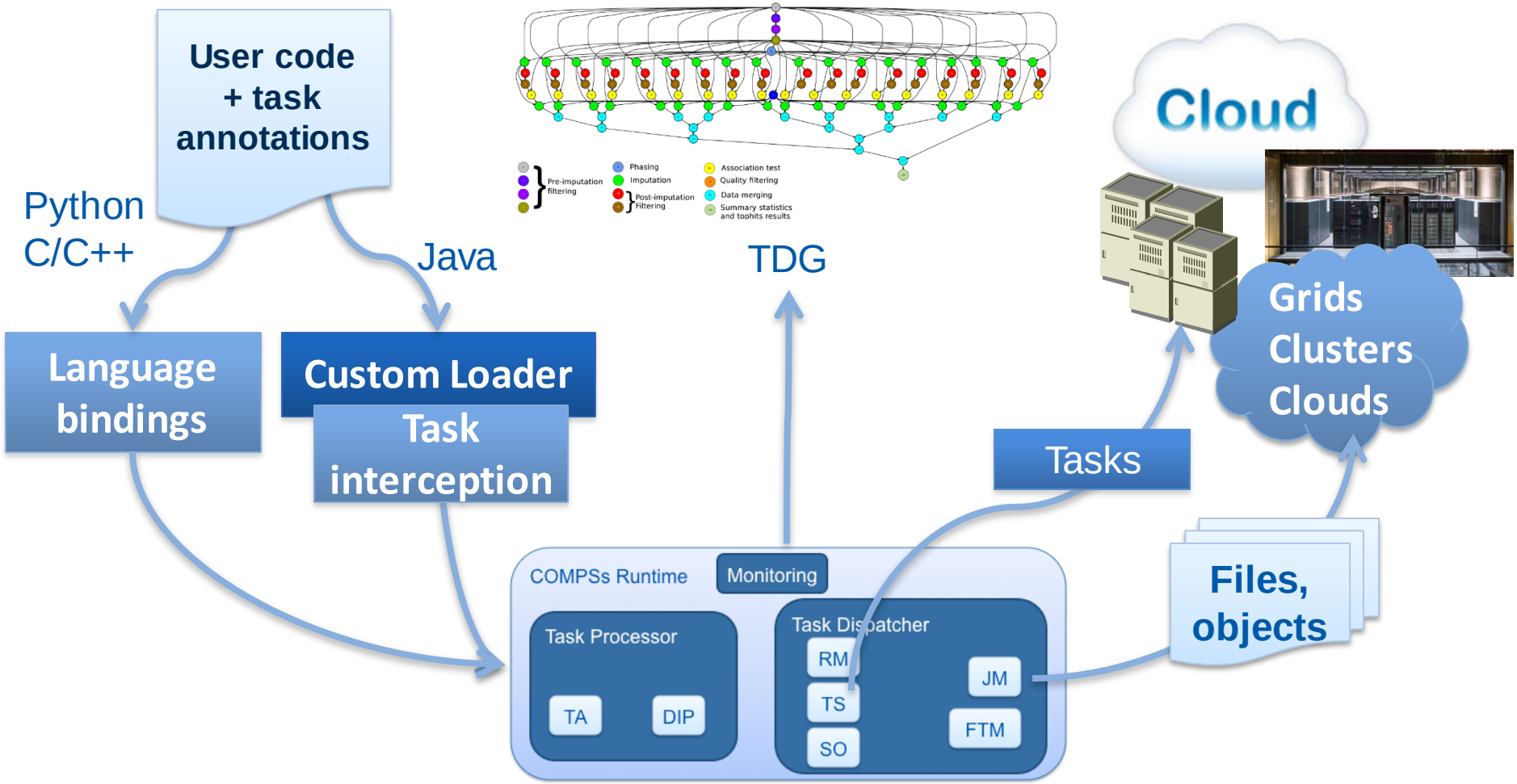


Programming with COMPSs

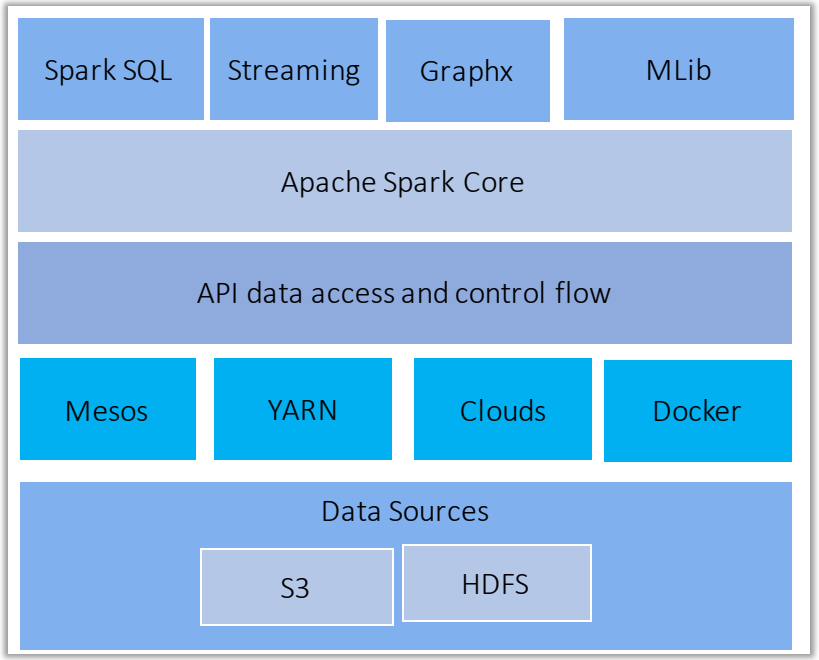
- Support for other types of parallelism
  - Threaded tasks (I.e., MKL kernels)
  - MPI applications -> tasks that involve several nodes
  - Integration with BSC OmpSs
- Available in MareNostrum, in the EGI Federated Cloud and in Chameleon Cloud

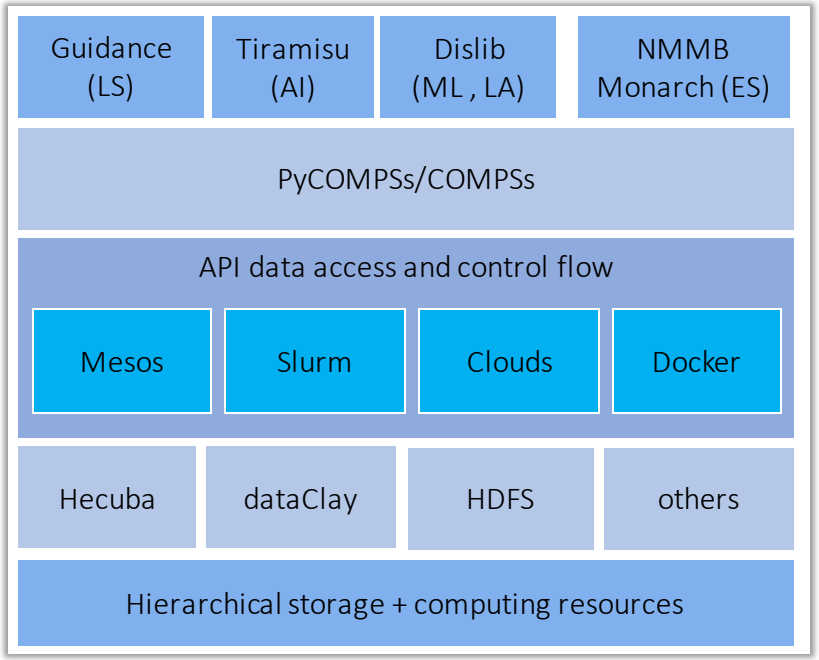


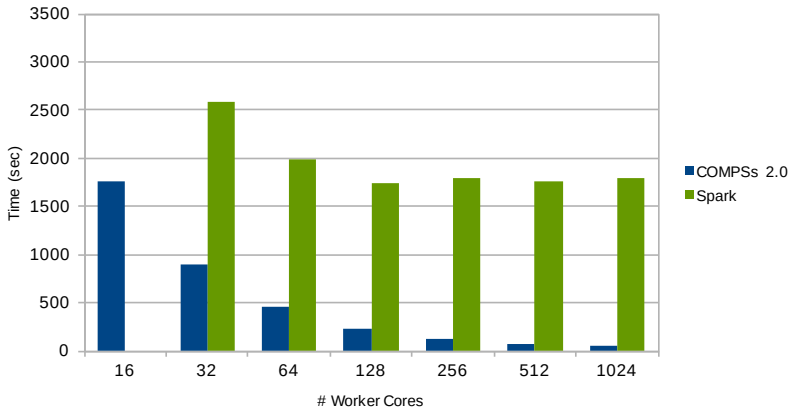
COMPSs Runtime

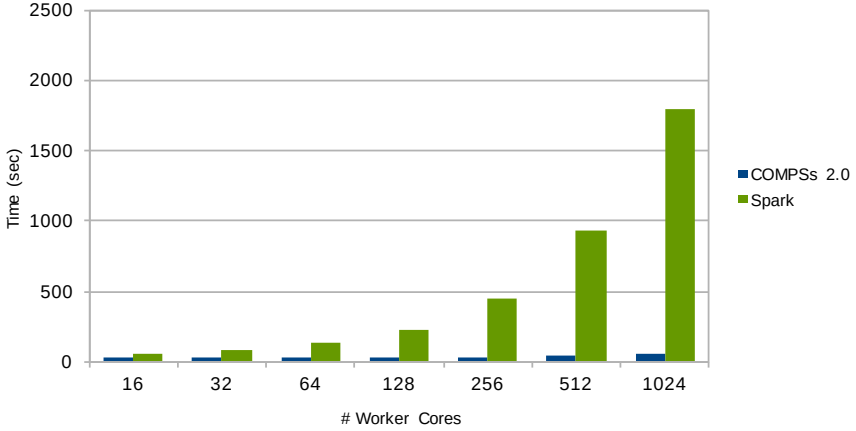


David vs Goliath



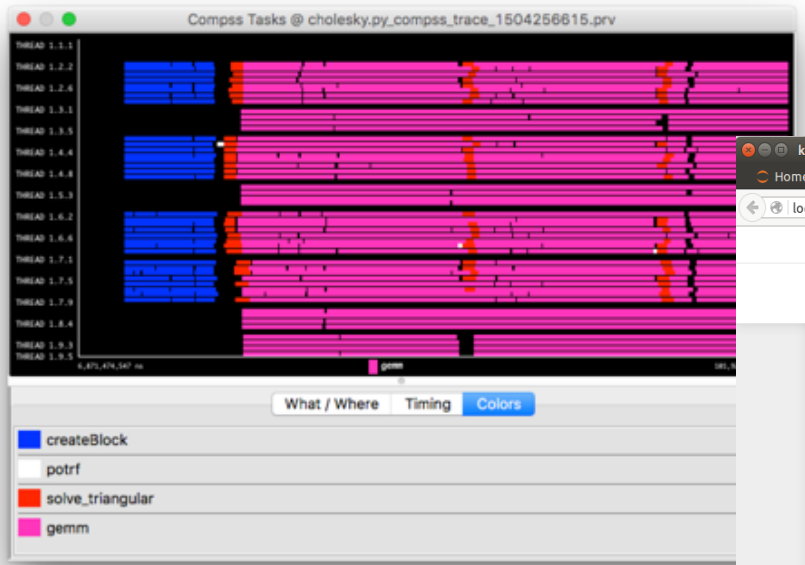


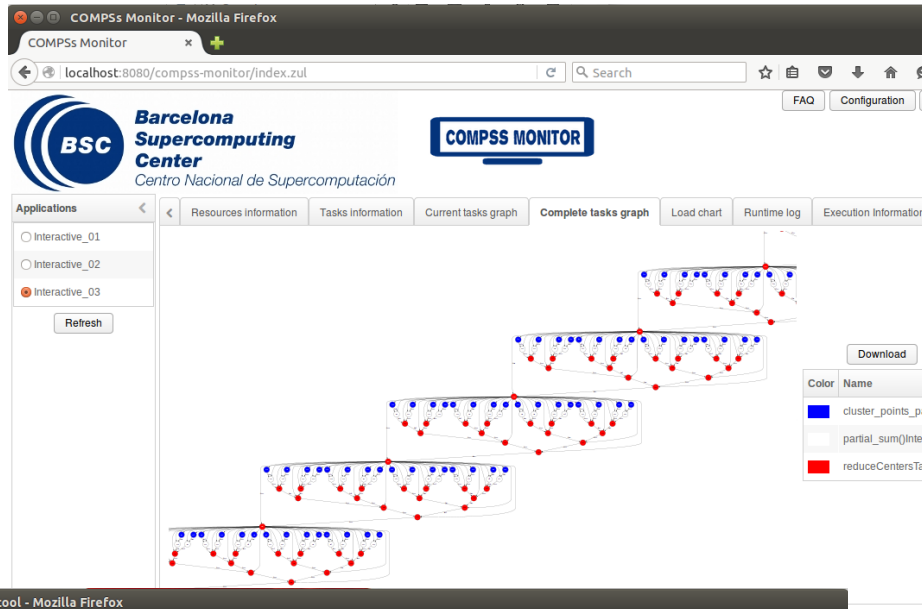


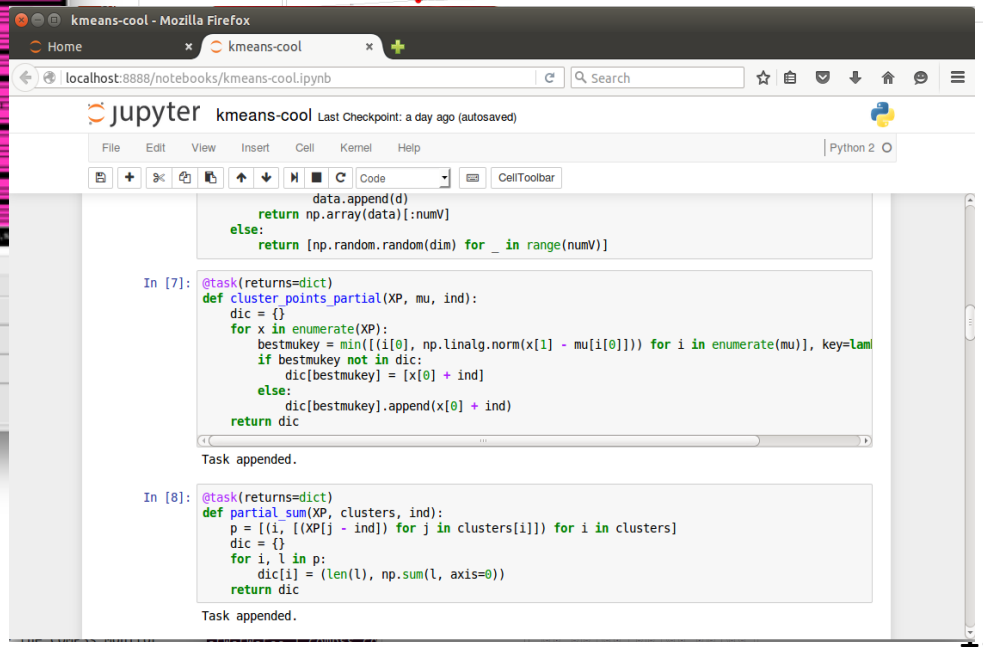


PyCOMPSs development environment

- Runtime monitor
- Paraver traces
- Jupyter-notebooks integration







Projects where COMPSs is used/developed

Multiscale Complex Genomics

mF2C

TANGO

bioexcel
Center of Excellence for Computational Biomolecular Research

CLASS

nextgenio

EXPERTISE

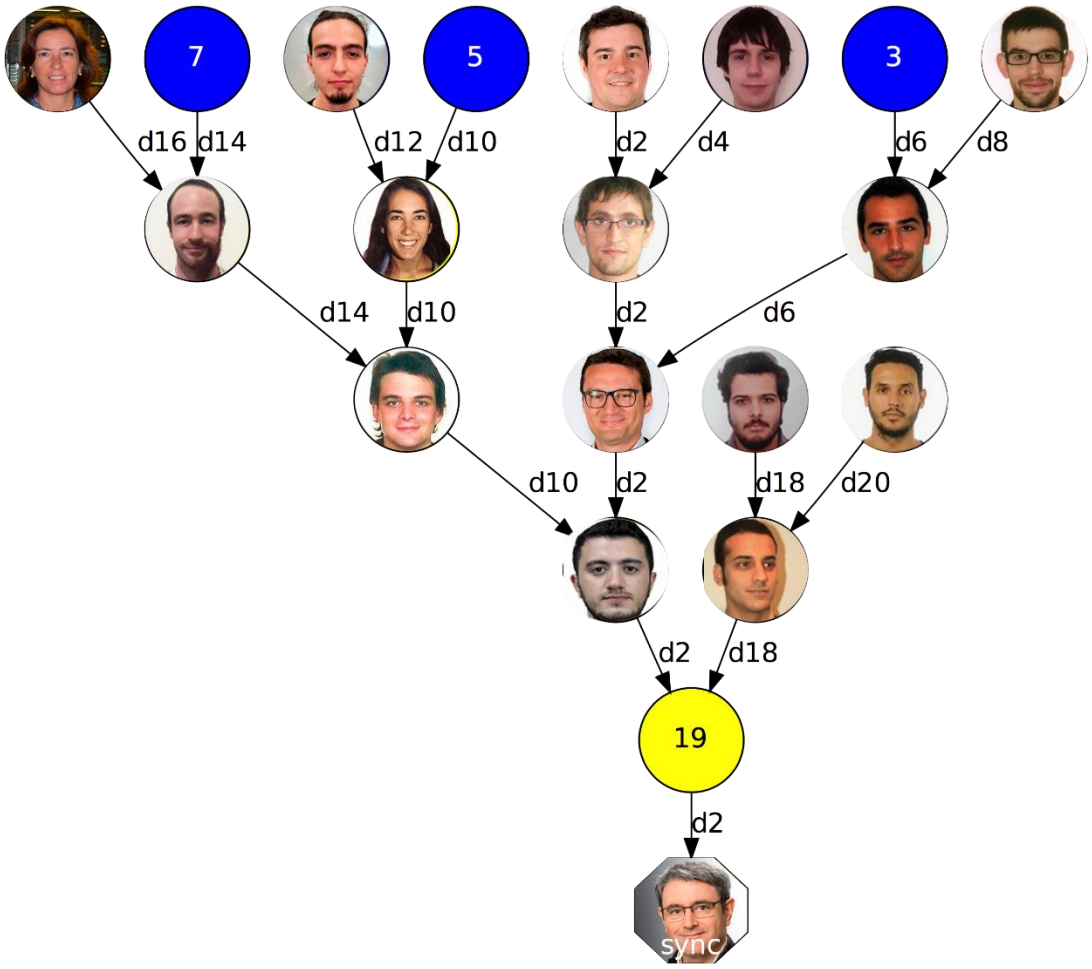
LANDSUPPORT

ExaQUte
Exascale Quantification of Uncertainties for Technology and Science Simulation

FUJITSU

BSC Barcelona Supercomputing Center
Centro Nacional de Supercomputación

The WDC team



http://compss.bsc.es

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SETUP OF THE TUTORIAL ENVIRONMENT

COMPSs docker

- Install Docker in your laptop
  - https://www.docker.com/products/docker-desktop
- Clone the examples apps

```
> git clone https://github.com/bsc-wdc/tutorial_apps.git
```

- COMPSs image downloadable from docker hub

```
> docker pull compss/compss-tutorial:patc2019
```

- Start the container

Laptop directory where you have the examples

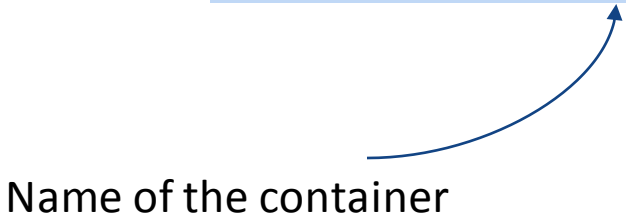
```
> docker run -p 8888:8888 -p 8080:8080 -v path/to/tutorial_apps:/home/tutorial_apps \
                -itd compss/compss-tutorial:patc2019 --name mycompss
```

Image directory where you will find the examples

PyCOMPSs docker

- Start interactive session in the Docker container

```
> docker exec -it  mycompss /bin/bash
```



PyCOMPSs docker

- Inside the image
  - Start the COMPSs monitor:

```
> /etc/init.d/compss-monitor start
```

  - Start Jupyter

```
> jupyter-notebook --no-browser --allow-root --ip=172.17.0.2 --NotebookApp.token=
```

PyCOMPSs docker

- From your browser
  - Open Jupyter notebooks interface

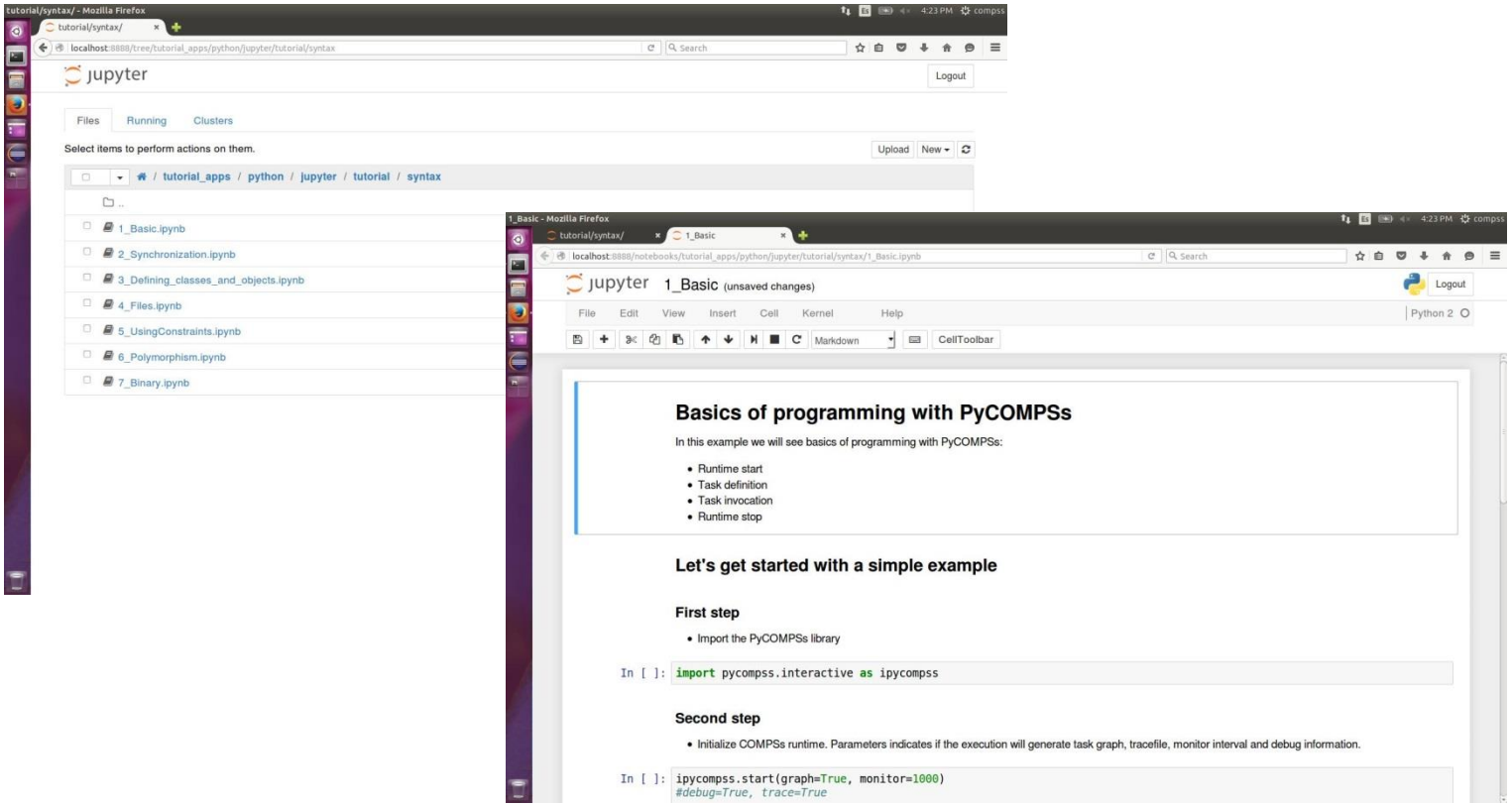
    http://localhost:8888/

  - Open COMPSs monitor

    http://localhost:8080/compss-monitor/index.zul

PyCOMPSs docker

- Ready to play with the notebooks



PYTHON SYNTAX

Why Python?

- Python is powerful... and fast;
  plays well with others;
  runs everywhere;
  is friendly & easy to learn;
  is Open. *

- Its design philosophy emphasizes code readability, and its syntax allows programmers to express concepts in fewer lines of code than would be possible in languages such as C
- Large community using it, including scientific and numeric
- Object-oriented programming and structured programming are fully supported
- Large number of software modules available (>127,000 as of January 2018) **

* From python.org ** From pypi.python.org